Triethylenetetramine
112-24-3 | DTXSID9023702

Model Performance

Model	Data

Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.89	0.25	0.88	0.26	0.75	0.38

Model Results

Predicted value: 3.68 days

Global applicability domain: Inside

Local applicability domain index: 6.32e-01

Confidence level: 8.25e-01

Nearest Neighbors from the Training Set

Image not found
2-Methyloctane
Measured: 40.7
Predicted: 4.23

Image not found
2-Methylheptane
Measured: 12.5
Predicted: 3.99

Image not found
2-Methylhexane
Measured: 12.5
Predicted: 5.54

Image not found
3-Methyloctane
Measured: 40.7
Predicted: 4.08